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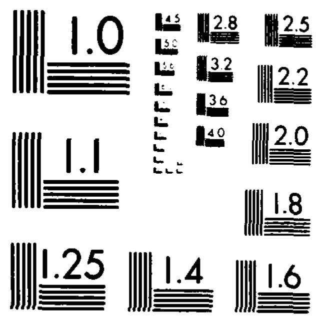

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SYNTHESIS AND CHARACTERIZATION OF A DIMERIC HYDRIDORHODACARBABORANE ANION DERIVED FROM THE *NIDO*-MONOCARBABORANE, $B_{10}H_{12}CNH_3$

By

John A. Walker, Conrad A. O'Con, Limin Zheng, Carolyn B. Knobler and M. Frederick Hawthorne*

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Department of Chemistry and Biochemistry
University of California
Los Angeles, California 90024

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Synthesis and Characterization of a Dimeric Hydridorhodacarbaborane Anion Derived from the *nido*-Monocarbaborane, $B_{10}H_{12}CNH_3$

By John A. Walker, Conrad A. O'Con, Limin Zheng, Carolyn B. Knobler and M. Frederick Hawthorne*

Department of Chemistry, University of California, Los Angeles, California 90024

Summary The reaction of $RhCl(PPh_3)_3$ with *nido*-$B_{10}H_{12}CNH_3$ in the presence of $[(n\text{-}C_4H_9)N]OH$ produced $[(n\text{-}C_4H_9)_4N][closo\text{-}2,2\text{-}(Ph_3P)_2\text{-}2\text{-}H\text{-}1\text{-}(NH_2)\text{-}2,1\text{-}RhCB_{10}H_{10}]$, which upon heating in methanol produced a new orange compound confirmed by an X-ray diffraction study to be the $[(n\text{-}C_4H_9)_4N]^+$ salt of an $-NH_2$-bridged Rh-H-Rh dimer anion.

The synthesis of catalytically active hydridorhodacarboranes via formal oxidative addition of the *nido*-carbaborane anions 7,8-,[1] 7,9-,[1a] and 2,9-[1b] $C_2B_9H_{12}$ to $RhCl(PPh_3)_3$ has been previously described. We now report the extension of this reaction to the *nido*-carbaborane anions derived from the *nido*-monocarbaborane, $B_{10}H_{12}CNH_3$.[2]

Treatment of $RhCl(PPh_3)_3$ with an equal molar quantity of *nido*-$B_{10}H_{12}CNH_3$ and three molar equivalents of potassium hydroxide in methanol produced a yellow solution of $K[closo\text{-}2,2\text{-}(PPh_3)_2\text{-}2\text{-}H\text{-}1\text{-}(NH_2)\text{-}2,1\text{-}RhCB_{10}H_{10}]$, K1. Metathesis of this salt with $[(n\text{-}C_4H_9)_4N]Br$ or PPNCl produced a bright yellow precipitate of the respective salt of 1^- (80% yield). The i.r.

spectrum (nujol mull) of [(n-$C_4H_9)_4N$] 1 displayed a medium intensity band at 2050 cm^{-} assigned to ν_{RhH}. The 200 mHz ^1H n.m.r. spectrum of freshly prepared d_6-acetone solutions of [(n-C_4H_9)N] 1 displayed a six line hydride resonance at -10.28 ppm consistent with the hydride ligand being coupled to ^{103}Rh and two equivalent ^{31}P nuclei. Additionally, the observation of a four line rhodium hydride resonance at -9.75 ppm indicates that 1^{-} dissociates one triphenylphosphine ligand in solution. In accord with this observation, the 81.02 mHz $^{31}P\{^1H\}$ n.m.r. spectrum of freshly prepared 10% d_6-acetone-acetone solutions of (n-$C_4H_9)_4N$] 1 displays two doublets centered at 35.3 ppm (J_{Rh-P}=139 Hz) and 34.2 ppm (J_{Rh-P}=112 Hz) and a singlet at -4.22 ppm. The singlet is assigned to uncoordinated triphenylphosphine and the lower field doublet is assigned to [(n-$C_4H_9)_4N$] 1. The higher field doublet is assigned to the monotriphenylphosphine species observed in the ^1H n.m.r. spectrum of this salt.

Heating a solution of [(n-$C_4H_9)_4N$] 1 in methanol at the reflux temperature for short periods produced a new ionic orange species [(n-$C_4H_9)_4N$] 2. This same species was directly produced in high yield from the reaction of nido-$B_{10}H_{12}CNH_3$ and $RhCl(PPh_3)_3$ and [(n-$C_4H_9)_4N$]OH in refluxing methanol and [$(C_2H_5)_3NH$] 2 is produced in high yield from nido-$B_{10}H_{12}CNH_3$, $RhCl(PPh_3)_3$ and triethylamine in refluxing methanol. Elemental analyses and osmometric molecular weight measurements on [$(C_2H_5)_3NH$] 2 established a Rh:P:B:N ratio of 1:1:10:1.5 and that this species was probably dimeric. The 81.02 MHz $^{31}P\{^1H\}$ n.m.r. spectrum of d_6-acetone solutions of [$(C_2H_5)_3NH$] 2

displayed one doublet centered at 40.3 ppm (J_{Rh-P} = 140 Hz). The 200 MHz ^1H n.m.r. spectrum of d_6-acetone solutions of this salt displayed a five line rhodium-hydride resonance at -9.84 which upon ^{31}P decoupling collapsed to a triplet. This data is consistent with the hydride ligand being coupled to two equivalent ^{103}Rh nuclei and two equivalent ^{31}P nuclei. As a bridging hydride ligand in $[(C_2H_5)_3NH]$ **2** was indicated from the ^1H n.m.r. spectrum of this salt it was of interest to establish the exact coordination geometry of this species by x-ray crystallography since hydride ligands bridging two transition metals have been heretofore unobserved in metallacarbaborane chemistry.

Poor solubility properties of $[(C_2H_5)_3NH]$ **2** frustrated attempts to grow single crystals of this salt. The $[(\underline{n}-C_4H_9)_4N]^+$ salt of $\mathbf{2}^-$ was more soluble in organic solvents which allowed red single crystals of $[(\underline{n}-C_4H_9)_4N]$ **2** to be grown from CH_2Cl_2-pentane.

Crystal data: M = 1308.659 {calcd. for $[(C_4H_9)_4N][P(Ph_3)RhCB_{10}H_{10}NH_2)_2H].1/2\ CH_2Cl_2$}, triclinic, space group $P\bar{1}$, $\underline{a}$ = 13.767(3), $\underline{b}$ = 14.618(3), $\underline{c}$ = 17.672(4) Å, α= 95.65(2), β= 94.52(2), γ= 98.73(1)^o, $\underline{V}$ = 3482(1) Å^3, Z = 2; D_c = 1.25 g cm^{-3}; D_m = 1.27 g cm^{-3}; (aq KI); R is currently 0.063 for 8122 unique reflections having I > 3 σ(I) (Syntex $P\bar{1}$ four circle diffractometer, MoKalpha radiation, lambda = 0.7107 Å).

The structure of $\mathbf{2}^-$ is shown in the figure. Each Rh is symmetrically bonded to all five atoms of a CB_4 pentagonal face at distances ranging from 2.12-2.26 Å, and also to P of a single triphenylphosphine ligand (2.367(3) and 2.356(2) Å) and interacts

with the other monocarbollide ligand via the NH_2 group on C (2.221(6) and 2.220(6) Å). In addition, a single hydride atom bridges the two Rh atoms at distances of 1.92(7) and 1.90(7) Å, while the separation between the Rh atoms is 2.998(1) Å. The dimer possesses approximately 2-fold symmetry about an axis perpendicular to the Rh-Rh bond. The Rh-Rh bond length of $\underline{2}^-$ can be compared to 2.763(1) Å found in the Rh(II) dimer, $[(Ph_3P)\text{-}RhC_2B_9H_{11}]_2$[3] and to 2.906(1) Å found in the Rh(III) dimer $[(\mu\text{-}H)(\mu\text{-}Cl)\{(\eta\text{-}C_5(CH_3)_5\text{-}RhCl\}_2]$.[4] The Rh-H-Rh distances cited above compare to 1.805(4) and 1.812(3) Å found in $\{HRh[P(o\text{-}\underline{i}\text{-}C_3H_7)_3]_2\}_2$.[5]

The exact mode of formation of $\underline{2}^-$ from $\underline{1}^-$ was not determined but probably follows the pathway indicated in Scheme I. The spectroscopically observable intermediate A is unstable with respect to bimolecular reductive elimination of molecular hydrogen forming the undetected dimeric intermediate B. Similar dimer formation from the putative monometallic 16 electron rhodium hydride species $3\text{-}(Ph_3P)\text{-}3\text{-}H\text{-}1\text{-}(\underline{n}\text{-}C_4H_9)\text{-}3,1,2\text{-}RhC_2B_9H_{11}$ has been previously reported.[6] In the present case, dimer formation is further promoted by the presence of the nucleophilic amino substituents on the carbaborane ligand. The dinegative intermediate B then abstracts a proton from the solvent yielding the observed monoanion, $\underline{2}^-$. The proposed protonation of B constitutes a formal two electron oxidation of the dinuclear Rh(II) species to the dinuclear Rh(III) product and $\underline{2}^-$ is the first isolated dimeric rhodacarbaborane with rhodium in the +3 oxidation state.

Other rhodacarbaboranes derived from $\underline{nido}\text{-}B_{10}H_{12}C\text{-}N(CH_3)_3$,

nido-$B_{10}H_{12}CH^-$ and *nido*-$CB_9PH_{11}^-$ have been isolated and characterized, some of which exhibit catalytic activity comparable to *closo*-3,3-$(PPh_3)_2$-3-H-3,1,2-$RhC_2B_9H_{11}$. The results of these studies will be presented elsewhere.[7]

Acknowledgements

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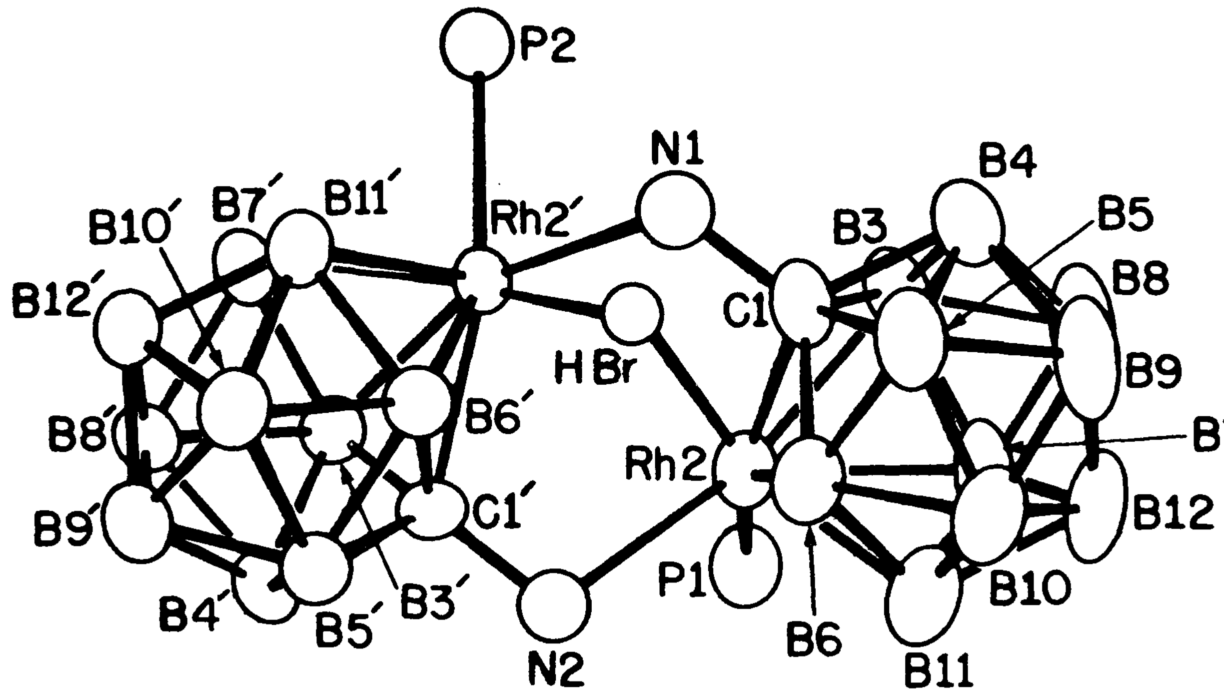
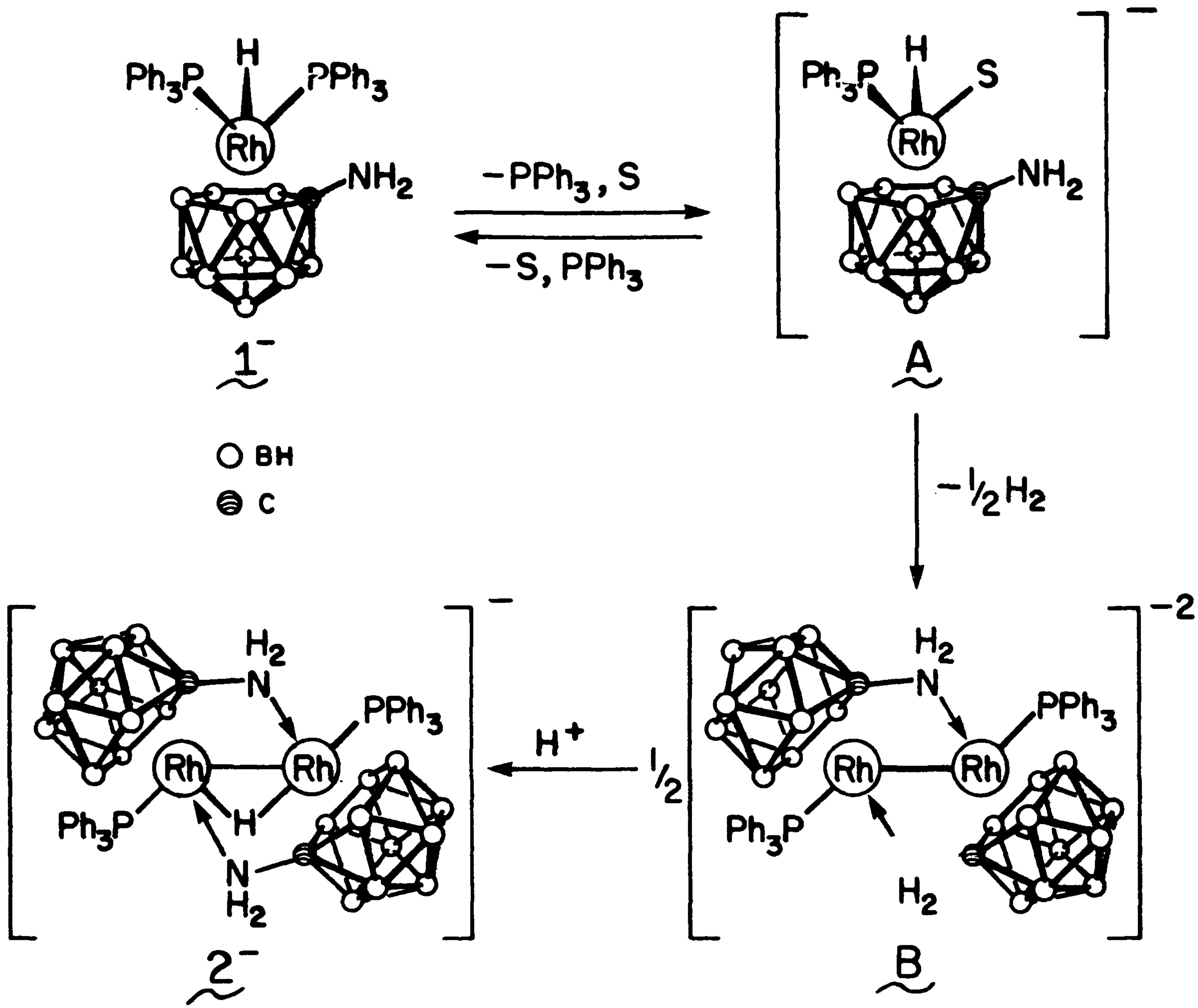
Figure Caption

An ORTEP projection of anion **2**. Thermal ellipsoids are shown at 50% probability. Phenyl groups and all hydrogen atoms except the bridging hydride have been omitted for clarity. Some distances are Rh(2)-B(3) 2.125(10), Rh(2)-B(6) 2.231(10), Rh(2)-B(7) 2.206(10), Rh(2)-B(11) 2.265(10), Rh(2)-C(1) 2.189(9), Rh(2')-B(3') 2.163(9), Rh(2')-B(6') 2.205(9), Rh(2')-B(7') 2.212(9), Rh(2')-B(11') 2.2551(9), Rh(2')-C(1') 2.178(7) Å. Some angles are P(1)-Rh(2)-H(Br) 83(2), N(2)-Rh(2)-H(Br) 94(2), B(11)-Rh(2)-H(Br) 164(2), N(2)-Rh(2)-P(1) 93.8(2), P(1)-Rh(2)-Rh(2') 112.80(6), P(2)-Rh(2')-H(Br) 84(2), N(1)-Rh(2')-H(Br) 83(2), B(11')-Rh(2')-H(Br) 174(2), N(1)-Rh(2')-P(2) 88.4(2), P(2)-Rh(2')-Rh(2) 117.24(6)°.


P2
N1
B4
B11´
B7´
Rh2´
B10´
B3
B5
B12´
B8
C1
H Br
B9
B8´
B6´
B7
Rh2
B9´
C1´
B12
P1
B10
B4´
B3´
B5´
B6
N2
B11


Ph3P
H
PPh3
Rh
NH2
1⁻
BH
C
−PPh3, S
−S, PPh3
Ph3P
H
S
Rh
NH2
A
−1/2 H2
H2
N
PPh3
Rh
Rh
Ph3P
H2
B
−2
1/2
H+
H2
N
PPh3
Rh
Rh
Ph3P
H
N
H2
2⁻

POSITIONAL PARAMETERS

ATOM	X		Y		Z	
[illegible](3')	0.1688(	7)	0.1957(	6)	[illegible]	[illegible]
[illegible](3)	0.2536(	8)	0.1931(	7)	0.417[illegible]	[illegible]
[illegible](4')	0.1930(	7)	0.3048(	7)	0.0[illegible]	[illegible]
[illegible](4)	0.3746(	9)	0.2457(	5)	[illegible]	[illegible]
[illegible](5')	0.2641(	7)	0.3872(	6)	[illegible]	[illegible]
[illegible](5)	0.4031(	9)	0.3604(	9)	0.4[illegible]	[illegible]
[illegible](6')	0.3428(	7)	0.3325(	6)	[illegible]	[illegible]
[illegible](6)	0.[illegible]010(	9)	0.2781(	7)	0.3[illegible]	[illegible]
[illegible](7')	0.[illegible]738(	7)	0.1535(	7)	0.0[illegible]	[illegible]
[illegible](7)	0.1660(	9)	0.2615(	8)	0.4[illegible]	[illegible]
[illegible](8')	0.1938(	7)	0.2123(	7)	0.0[illegible]	[illegible]
[illegible](8)	0.2701(	10)	0.2439(	9)	[illegible]	[illegible]
[illegible](9')	0.2521(	8)	0.3298(	7)	[illegible]	[illegible]
[illegible](9)	0.3589(	11)	0.3460(	10)	[illegible]	[illegible]
[illegible](10')	0.3653(	7)	0.3462(	[illegible])	0.07[illegible]	[illegible]
[illegible](10)	0.3161(	10)	0.4249	[illegible]	0.4[illegible]	[illegible]
[illegible](11')	0.3342(	7)	0.2401(	7)	[illegible]	[illegible]
[illegible](11)	0.1931(	9)	0.3792(	8)	[illegible]	[illegible]
[illegible](12')	0.3235(	7)	0.2394(	7)	[illegible]	[illegible]
[illegible](12)	0.2350(	10)	0.3554(	9)	[illegible]	[illegible]
[illegible](1')	0.2155(	5)	0.3046(	5)	[illegible]	[illegible]
[illegible](1)	0.[illegible]242(	7)	0.2609(	6)	[illegible]	[illegible]
[illegible](C11)	0.5140(	9)	0.3971(	8)	[illegible]	[illegible]
[illegible](C12)	0.5691(	9)	0.3316(	9)	0.9010[illegible]	[illegible]
[illegible](C13)	0.6311(	10)	0.3769(	10)	0.9[illegible]	[illegible]
[illegible](C14)	0.6794(	15)	0.3259(	17)	1.0[illegible]	[illegible]
[illegible](C21)	0.3668(	9)	0.2917(	9)	0.8[illegible]	[illegible]
[illegible](C22)	0.2907(	14)	0.2565(	12)	0.74[illegible]	[illegible]
[illegible](C23)	0.2072(	28)	0.1243(	21)	0.77[illegible]	[illegible]
[illegible](C24)	0.2552(	24)	0.1067(	24)	0.75[illegible]	[illegible]
[illegible](C31)	0.4168(	12)	0.4425(	9)	0.75[illegible]	[illegible]
[illegible](C32)	0.[illegible]578(	15)	0.4754(	12)	[illegible]	[illegible]
[illegible](C33)	0.[illegible]076(	22)	0.5674(	14)	0.750[illegible]	[illegible]
[illegible](C34)	0.3263(	24)	0.6449(	17)	0.7[illegible]	[illegible]
[illegible](C41)	0.5145(	9)	0.3126(	9)	0.77[illegible]	[illegible]
[illegible](C42)	0.6004(	12)	0.3682(	12)	0.71[illegible]	[illegible]
[illegible](C43)	0.[illegible]551(	15)	0.3103(	12)	0.6[illegible]	[illegible]
[illegible](C44)	0.7535(	16)	0.3473(	[illegible])	[illegible]	[illegible]
N(1)	0.3883(	5)	0.2331(	4)	0.31[illegible]	[illegible]
N(2)	0.1599(	5)	0.337[illegible](	4)	0.22[illegible]	[illegible]
N(C01)	0.1541(	6)	0.3618(	5)	[illegible]	[illegible]
P(1)	0.0122(	2)	0.1887(	2)	[illegible]	[illegible]
P(2)	0.3271(	2)	0.0396(	1)	0.205[illegible]	[illegible]
RH(2')	0.28845(	4)	0.19037(	4)	0.2650[illegible]	[illegible]
RH(2)	0.17996(	5)	0.2595[illegible](	4)	0.33[illegible]	[illegible]
[illegible]BR	0.1749(	54)	0.1476(	50)	[illegible]	[illegible]
[illegible]B 3'	0.0970		0.1644		0.1[illegible]	
[illegible]B 3)	0.2577		0.1051		0.410	
[illegible]B [illegible]	0.0381		0.3266		0.0759	
[illegible]B 4)	0.4392		0.2023		0.4[illegible]	
[illegible]B [illegible]	0.[illegible]677		0.4617		0.1[illegible]	
[illegible]B [illegible]	0.4[illegible]		0.[illegible]742		0.4[illegible]	
[illegible]B 6'	0.[illegible]814		0.3704		[illegible]	
[illegible]B 6)	0.[illegible]		0.4[illegible]		[illegible]	
[illegible]	0.[illegible]673		0.0[illegible]		[illegible]	
[illegible]	0.[illegible]52		0.[illegible]4		[illegible]	
[illegible]	[illegible]		0.1[illegible]		[illegible]	
[illegible]	[illegible]		[illegible]		[illegible]	

H(B 9)	0.2532	0.3905	-0.0346
H(B 9)	0.4135	0.3559	0.56[illegible]
H(B10)	0.4319	0.3947	0.0740
H(B10)	0.3183	0.4956	0.4797
H(B11)	0.4553	0.2223	0.110[illegible]
H(B11)	0.1266	0.4361	0.41[illegible]4
H(B12)	0.3633	0.2065	-0.03[illegible]
H(B12)	0.1850	0.3733	0.5604
H(C11)	0.5664	0.4627	0.6[illegible]
H(C11)	0.4784	0.4316	0.8998
H(C12)	0.6238	0.3105	0.8611
H(C12)	0.5160	0.2875	0.9218
H(C13)	0.5917	0.4186	1.0028
H(C14)	0.7057	0.3215	1.0[illegible]18
H(C14)	0.6897	0.2682	0.9685
H(C21)	0.3986	0.2310	0.8246
H(C34)	0.3842	0.6456	0.8076
H(C41)	0.4600	0.2881	0.6069
H(C42)	0.4515	0.3512	0.75[illegible]2
H(N1A)	0.4534	0.2685	0.2002
H(N1B)	0.4108	0.1763	0.3019
H(N2A)	0.1822	0.4026	0.2[illegible]4[illegible]
H(N2B)	0.0890	0.3250	0.2[illegible]

ISOTROPIC TEMPERATURE FACTORS

ATOM	UX10E 4	
N(1)	459(	16)
N(2)	453(	16)
N(C01)	658(	21)
DU	0	
H(B 3'	887	
H(B 3)	887	
H(B 4'	887	
H(B 4)	887	
H(B 5'	887	
H(B 5)	887	
H(B 6'	887	
H(B 6)	887	
H(B 7'	887	
H(B 7)	887	
H(B 8'	887	
H(B 8)	887	
H(B 9'	887	
H(B 9)	887	
H(B10'	887	
H(B10)	887	
H(B11'	887	
H(B11)	887	
H(B12'	887	
H(B12)	887	
H(BR)	253	
H(C11)	633	
H(C11)	633	
H(C12)	633	
H(C12)	633	
H(C13)	633	
H(C14)	1140	
H(C14)	1140	
H(C21)	633	
H(C34)	1140	
H(C41)	633	
H(C42)	633	
H(N1A)	633	
H(N1B)	633	
H(N2A)	887	
H(N2B)	887	

The complete temperature factor is
exp[-U*sin(theta>2<)/(lambda>2<8pi>2<)] or
exp[-B*sin(theta>2<)/lambda>2<)] where
B = U/8pi>2<.

ANISOTROPIC TEMPERATURE FACTORS

ATOM	U11X10E4	U22X10E4	U33X10E4	U12X10E4	U13X10E4	U2310E4
B(3')	416(53)	420(51)	365(40)	109(42)	13(40)	37(39)
B(3)	701(74)	647(60)	382(54)	99(57)	-17(50)	167(49)
B(4')	477(58)	503(57)	408(51)	101(45)	52(43)	150(43)
B(4)	862(87)	693(74)	416(58)	132(64)	-126(57)	45(52)
B(5')	549(61)	396(52)	495(56)	73(45)	164(47)	135(43)
B(5)	822(86)	650(72)	491(63)	-52(63)	-97(58)	-39(54)
B(6')	425(54)	396(50)	414(50)	-2(41)	103(41)	70(40)
B(6)	820(79)	393(54)	413(55)	0(52)	22(52)	-81(43)
B(7')	450(56)	529(57)	316(46)	59(45)	11(40)	80(41)
B(7)	866(86)	706(75)	353(54)	67(63)	129(54)	105(50)
B(8')	483(59)	566(61)	401(52)	159(48)	50(44)	113(45)
B(8)	1065(106)	965(98)	330(58)	-120(80)	-15(62)	94(60)
B(9')	553(64)	599(64)	437(55)	129(51)	118(47)	159(48)
B(9)	1211(121)	995(102)	346(60)	12(87)	-45(67)	-41(61)
B(10')	552(63)	424(54)	451(54)	36(46)	112(47)	37(43)
B(10)	1110(104)	593(71)	443(61)	40(69)	-20(64)	-139(52)
B(11')	402(54)	514(57)	447(53)	53(44)	112(42)	110(44)
B(11)	942(91)	561(67)	457(60)	15(62)	152(59)	-105(50)
B(12')	498(59)	502(58)	422(53)	62(46)	112(45)	115(44)
B(12)	1063(107)	826(88)	410(61)	67(76)	195(65)	-106(58)
C(1')	397(45)	324(40)	440(44)	79(34)	78(35)	56(34)
C(1)	668(60)	517(51)	330(43)	76(44)	-53(40)	15(37)
C(C11)	984(87)	918(83)	628(66)	150(68)	2(61)	-170(59)
C(C12)	860(85)	1176(100)	758(77)	217(74)	4(65)	139(71)
C(C13)	1051(101)	1644(132)	671(77)	568(93)	-156(71)	-63(80)
C(C14)	2172(211)	3597(304)	1020(125)	1803(214)	-659(127)	-448(152)
C(C21)	910(91)	1129(99)	985(93)	-180(76)	-250(74)	253(77)
C(C22)	1856(182)	1562(153)	1330(144)	-560(134)	-664(132)	354(117)
C(C23)	2153(330)	2161(310)	1800(242)	-890(274)	-1164(231)	571(259)
C(C24)	1015(322)	3001(472)	2365(308)	-1581(332)	-950(262)	1316(375)
C(C31)	1566(137)	868(92)	1102(105)	376(92)	-62(95)	97(78)
C(C32)	2162(200)	1459(150)	1449(140)	922(142)	-356(134)	-164(120)
C(C33)	3145(332)	1141(145)	1791(196)	654(198)	-471(193)	240(155)
C(C34)	3076(380)	1629(199)	1800(217)	-248(257)	-1292(223)	697(194)
C(C41)	1043(96)	1113(97)	546(64)	43(77)	-17(63)	-118(62)
C(C42)	1397(138)	1772(159)	925(103)	-518(120)	212(96)	124(101)
C(C43)	1849(186)	1412(146)	1745(168)	282(132)	1102(153)	-121(120)
C(C44)	1893(209)	2424(241)	1885(195)	769(182)	889(172)	709(169)
P(1)	573(15)	608(15)	444(13)	120(12)	152(11)	135(11)
P(2)	471(13)	398(12)	412(11)	80(10)	9(10)	28(9)
RH(2')	404(4)	361(4)	318(3)	57(3)	34(3)	41(3)
RH(2)	594(5)	405(4)	309(3)	76(3)	84(3)	42(3)

The complete temperature factor is exp[-2pi>2<(a>*<>2<U<11>h>2< +
b>*<>2<U<22>k>2< + c>*<>2<U<33>l>2< + 2a>*<b>*<U<12>hk +
2a>*<c>*<U<13>hl + 2b>*<c>*<U<23>kl)].

POSITIONAL PARAMETERS FOR GROUP ATOMS

ATOM	X	Y	Z
C(S1)	0.0665	0.4274	0.8192
CL(2)	0.0286	0.4794	0.9045
CL(1)	0.0030	0.4725	0.7438
H(S1)	0.1389	0.4489	0.8184
H(S2)	0.0434	0.3587	0.8152
C(11)	-0.0511	0.1678	0.2262
C(12)	-0.0751	0.2457	0.1945
C(13)	-0.1210	0.2365	0.1204
C(14)	-0.1428	0.1493	0.0782
C(15)	-0.1188	0.0713	0.1099
C(16)	-0.0729	0.0806	0.1840
H(12)	-0.0595	0.3084	0.2248
H(13)	-0.1382	0.2925	0.0977
H(14)	-0.1757	0.1426	0.0251
H(15)	-0.1344	0.0086	0.0797
H(16)	-0.0557	0.0245	0.2068
C(21)	-0.0855	0.2407	0.3690
C(22)	-0.0652	0.3248	0.4159
C(23)	-0.1417	0.3626	0.4477
C(24)	-0.2382	0.3163	0.4326
C(25)	-0.2585	0.2322	0.3858
C(26)	-0.1820	0.1944	0.3540
H(22)	0.0042	0.3581	0.4267
H(23)	-0.1270	0.4230	0.4813
H(24)	-0.2930	0.3434	0.4555
H(25)	-0.3278	0.1988	0.3749
H(26)	-0.1966	0.1339	0.3203
C(31)	-0.0027	0.0722	0.3565
C(32)	0.0489	0.0072	0.3221
C(33)	0.0361	-0.0835	0.3416
C(34)	-0.0282	-0.1092	0.3954
C(35)	-0.0798	-0.0443	0.4298
C(36)	-0.0670	0.0464	0.4103
H(32)	0.0951	0.0258	0.2834
H(33)	0.0732	-0.1301	0.3168
H(34)	-0.0374	-0.1743	0.4094
H(35)	-0.1260	-0.0627	0.4685
H(36)	-0.1041	0.0931	0.4351
C(41)	0.2303	-0.0580	0.1704
C(42)	0.2436	-0.1492	0.1780
C(43)	0.1680	-0.2226	0.1515
C(44)	0.0793	-0.2048	0.1176
C(45)	0.0660	-0.1136	0.1100
C(46)	0.1415	-0.0402	0.1364
H(42)	0.3074	-0.1620	0.2024
H(43)	0.1777	-0.2881	0.1570
H(44)	0.0251	-0.2574	0.0986
H(45)	0.0023	-0.1007	0.0856
H(46)	0.1320	0.0254	0.1310
C(51)	0.3695	-0.0014	0.2983
C(52)	0.4667	-0.0108	0.3195
C(53)	0.4902	-0.0473	0.3872
C(54)	0.4165	-0.0744	0.4336
C(55)	0.3194	-0.0650	0.4125
C(56)	0.2959	-0.0285	0.3448
H(52)	0.5196	0.0087	0.2861
H(53)	0.5600	-0.0539	0.4023
H(54)	0.4334	-0.1005	0.4822

H(55)	0.2664	-0.0845	0.4458
H(56)	0.2260	-0.0218	0.3296
C(61)	0.4343	0.0200	0.1511
C(62)	0.4313	-0.0563	0.0968
C(63)	0.5166	-0.0718	0.0635
C(64)	0.6046	-0.0110	0.0845
C(65)	0.6075	0.0652	0.1387
C(66)	0.5223	0.0807	0.1720
H(62)	0.3680	-0.1000	0.0818
H(63)	0.5144	-0.1266	0.0246
H(64)	0.6657	-0.0222	0.0606
H(65)	0.6707	0.1089	0.1539
H(66)	0.5244	0.1356	0.2110

INTERATOMIC DISTANCES

FROM	TO	DISTANCE
B(3')	H(B 3'	1.086
B(3')	C(1')	1.772(11)
B(3')	B(8')	1.783(12)
B(3')	B(4')	1.807(12)
B(3')	B(7')	1.819(13)
B(3')	RH(2')	2.163(9)
B(3)	H(B 3)	1.290
B(3)	C(1)	1.749(13)
B(3)	B(8)	1.790(14)
B(3)	B(4)	1.806(16)
B(3)	B(7)	1.819(16)
B(3)	RH(2)	2.125(10)
B(4')	H(B 4'	1.060
B(4')	C(1')	1.730(11)
B(4')	B(9')	1.766(13)
B(4')	B(5')	1.768(13)
B(4')	B(8')	1.771(13)
B(4)	H(B 4)	1.169
B(4)	C(1)	1.690(12)
B(4)	B(8)	1.780(18)
B(4)	B(9)	1.789(17)
B(4)	B(5)	1.791(16)
B(5')	H(B 5'	1.096
B(5')	C(1')	1.734(11)
B(5')	B(10')	1.738(13)
B(5')	B(9')	1.779(13)
B(5')	B(6')	1.789(13)
B(5)	H(B 5)	1.090
B(5)	C(1)	1.722(13)
B(5)	B(10)	1.750(17)
B(5)	B(6)	1.761(16)
B(5)	B(9)	1.762(16)
B(6')	H(B 6'	1.054
B(6')	C(1')	1.733(11)
B(6')	B(10')	1.756(12)
B(6')	B(11')	1.796(13)
B(6')	RH(2')	2.205(9)
B(6)	H(B 6)	1.018
B(6)	C(1)	1.738(13)
B(6)	B(10)	1.747(13)
B(6)	B(11)	1.830(16)
B(6)	RH(2)	2.231(10)
B(7')	H(B 7'	1.202
B(7')	B(8')	1.792(13)
B(7')	B(12')	1.793(13)
B(7')	B(11')	1.847(13)
B(7')	RH(2')	2.212(9)
B(7)	H(B 7)	1.226
B(7)	B(8)	1.758(18)
B(7)	B(12)	1.777(16)
B(7)	B(11)	1.841(15)
B(7)	RH(2)	2.206(10)
B(8')	H(B 8'	1.347
B(8')	B(12')	1.774(13)
B(8')	B(9')	1.709(14)
B(8)	H(B 8)	1.190
B(9)	B([illegible])	1.765(19)
B(9)	B(4)	1.786(18)

B(9')	H(B 9')	1.392
B(9')	B(12')	1.763(14)
B(9')	B(10')	1.773(14)
B(9)	H(B 9)	0.977
B(9)	B(10)	1.710(18)
B(9)	B(12)	1.729(20)
B(10')	H(B10')	1.029
B(10')	B(12')	1.774(13)
B(10')	B(11')	1.775(13)
B(10)	H(B10)	1.025
B(10)	B(12)	1.756(17)
B(10)	B(11)	1.794(17)
B(11')	H(B11')	1.049
B(11')	B(12')	1.790(13)
B(11')	RH(2')	2.251(9)
B(11)	H(B11)	1.372
B(11)	B(12)	1.777(16)
B(11)	RH(2)	2.265(10)
B(12')	H(B12')	1.237
B(12)	H(B12)	1.272
C(1')	N(2)	1.452(9)
C(1')	RH(2')	2.178(7)
C(1)	N(1)	1.453(10)
C(1)	RH(2)	2.189(9)
C(C11)	H(C11)	0.979
C(C11)	H(C11)	1.192
C(C11)	C(C12)	1.479(15)
C(C11)	N(C01)	1.504(12)
C(C12)	H(C12)	1.010
C(C12)	H(C12)	1.128
C(C12)	C(C13)	1.503(15)
C(C13)	H(C13)	1.026
C(C13)	C(C14)	1.321(20)
C(C14)	H(C14)	0.729
C(C14)	H(C14)	1.154
C(C21)	H(C21)	1.107
C(C21)	C(C22)	1.458(17)
C(C21)	H(C01)	1.533(13)
C(C22)	C(C23)	1.568(37)
C(C23)	C(C24)	1.382(62)
C(C31)	C(C32)	1.450(20)
C(C31)	N(C01)	1.532(14)
C(C32)	C(C33)	1.617(24)
C(C33)	C(C34)	1.133(23)
C(C34)	H(C34)	1.007
C(C41)	H(C41)	1.060
C(C41)	C(C42)	1.413(16)
C(C41)	N(C01)	1.524(13)
C(C42)	H(C42)	0.975
C(C42)	C(C43)	1.566(20)
C(C43)	C(C44)	1.389(24)
N(1)	H(N1B)	1.011
N(1)	H(N1A)	1.012
N(1)	RH(2')	2.221(6)
N(2)	H(N2A)	0.955
N(2)	H(N2B)	1.025
N(2)	RH(2)	2.220(6)
P(1)	RH(2)	2.367(3)
P(2)	RH(2')	2.356(2)
RH(2')	H(BP)	1.923(71)
RH(2')	RH(2)	2.998(1)
RH(2)	H(BP)	1.905(71)
[illegible]	[illegible]	1.190

B(8)	B(12)	1.765(19)
B(8)	B(9)	1.766(18)
B(8)	H(B 9)	2.406
B(8)	H(B 7)	2.561
B(8)	H(B 3)	2.579
B(8)	H(B 4)	2.733
B(8)	H(B12)	2.752
B(8)	C(1)	2.769(14)
B(8)	B(10)	2.837(17)
B(8)	B(11)	2.899(18)
B(9')	H(B 9')	1.392
B(9')	B(12')	1.763(14)
B(9')	B(10')	1.773(14)
B(9')	H(B 4')	2.521
B(9')	H(B10')	2.562
B(9')	H(B 5')	2.598
B(9')	H(B 8')	2.673
B(9')	H(B12')	2.691
B(9')	C(1')	2.812(12)
B(9')	B(11')	2.908(14)
B(9)	H(B 9)	0.977
B(9)	B(10)	1.710(18)
B(9)	B(12)	1.729(20)
B(9)	H(B10)	2.523
B(9)	H(B 5)	2.605
B(9)	H(B 8)	2.610
B(9)	H(B 4)	2.716
B(9)	H(B12)	2.745
B(9)	C(1)	2.750(13)
B(9)	B(11)	2.863(19)
B(10')	H(B10')	1.029
B(10')	B(12')	1.774(13)
B(10')	B(11')	1.775(13)
B(10')	H(B11')	2.465
B(10')	H(B 5')	2.475
B(10')	H(B 6')	2.519
B(10')	H(B 9')	2.640
B(10')	H(B12')	2.705
B(10')	C(1')	2.768(12)
B(10')	H(C11)	2.943
B(10)	H(B10)	1.025
B(10)	B(12)	1.756(17)
B(10)	B(11)	1.794(17)
B(10)	H(B 9)	2.446
B(10)	H(B 6)	2.493
B(10)	H(B12)	2.634
B(10)	H(B 5)	2.658
B(10)	H(B11)	2.754
B(10)	C(1)	2.767(13)
B(11')	H(B11')	1.049
B(11')	B(12')	1.790(13)
B(11')	ZN(2')	2.251(9)
B(11')	H(B10')	2.341
B(11')	H(B 6')	2.575
B(11')	H(B12')	2.596
B(11')	H(B 7')	2.759
B(11')	C(1')	2.860(12)
B(11)	H(B11)	1.372
B(11)	B(12)	1.777(16)
B(11)	[illegible]	2.265(10)
B(11)	H(B10)	2.287
B(11)	[illegible]	2.488
B(11)	H(B 6)	2.568

B(11)	H(B 7)	2.744	
B(11)	C(1)	2.890(	15
B(12')	H(B12'	1.237	
B(12')	H(B11'	2.453	
B(12')	H(B10'	2.480	
B(12')	H(B 7'	2.611	
B(12')	H(B 8'	2.732	
B(12')	H(B 9'	2.780	
B(12)	H(B12)	1.272	
B(12)	H(B10)	2.403	
B(12)	H(B 9)	2.516	
B(12)	H(B 8)	2.597	
B(12)	H(B 7)	2.625	
B(12)	H(B11)	2.785	
C(1')	N(2)	1.452(	[illegible]
C(1')	H(N2A)	1.952	
C(1')	H(N2B)	1.967	
C(1')	RH(2')	2.178(	[illegible]
C(1')	H(B 6	2.406	
C(1')	H(B 3'	2.423	
C(1')	H(B 4'	2.431	
C(1')	[illegible]	2.479	
C(1')	H(BR)	3.046(	[illegible]
C(1')	RH(2	3.049(	[illegible]
C(1)	N(1)	1.453(	1[illegible]
C(1)	H(N1B)	2.085	
C(1)	H(N1A)	2.153	
C(1)	RH(2)	2.189(	[illegible]
C(1)	H(B 5)	2.330	
C(1)	H(B 4)	2.364	
C(1)	H(B 6)	2.381	
C(1)	H(B 3)	2.610	
C(1)	H(BR)	2.795(	7
C(1)	RH(2')	3.069(	[illegible]
C(C11)	H(C11)	0.979	
C(C11)	H(C11)	1.192	
C(C11)	C(C12)	1.479(	[illegible]
C(C11)	C(C31)	1.504(	[illegible]
C(C11)	H(C12)	1.980	
C(C11)	[illegible]	2.115	
C(C11)	C(C21)	2.332(	16
C(C11)	[illegible]	2.480(	17
C(C11)	C(C31)	2.492(	17
C(C11)	C(C41)	2.502(	1[illegible]
C(C11)	H(C13)	2.586	
C(C11)	H(C21)	2.689	
C(C11)	H(C42)	2.806	
C(C11)	C(C32)	2.973(	21
C(C11)	C(C42)	3.018(	19
C(C12)	H(C12)	1.010	
C(C12)	H(C12)	1.128	
C(C12)	C(C13)	1.503(	15
C(C12)	H(C11)	2.061	
C(C12)	H(C13)	2.085	
C(C12)	H(C11)	2.234	
[illegible]	H(C14)	2.326	
C(C12)	C(C14)	2.445(	19
[illegible]	[illegible]	2.5[illegible]	1[illegible]
[illegible]	[illegible]	2.7[illegible]0	
[illegible]	[illegible]	2.97[illegible]	[illegible]
[illegible]	[illegible]	2.998	
[illegible]	[illegible]	[illegible]	1[illegible]
[illegible]	[illegible]	[illegible]	

C(C13) C(C14)	1.321(	20)
C(C13) H(C14)	1.885	
C(C13) H(C14)	1.979	
C(C13) H(C12)	1.988	
C(C13) H(C12)	2.096	
C(C13) H(C11)	2.646	
C(C13) H(C11)	2.814	
C(C14) H(C14)	0.729	
C(C14) H(C14)	1.154	
C(C14) H(C12)	1.962	
C(C14) H(C12)	2.643	
C(C14) H(C12)	2.748	
C(C21) H(C21)	1.107	
C(C21) C(C22)	1.458(	17)
C(C21) N(C01)	1.533(	13)
C(C21) C(C41)	2.497(	18)
C(C21) C(C23)	2.499(	32)
C(C21) C(C31)	2.513(	19)
C(C21) H(C41)	2.574	
C(C21) H(C11)	2.686	
C(C21) H(C12)	2.774	
C(C21) C(C24)	2.894(	30)
C(C21) C(C32)	3.016(	22)
C(C22) C(C23)	1.568(	37)
C(C22) H(C21)	2.071	
C(C22) C(C24)	2.177(	35)
C(C22) N(C01)	2.546(	18)
C(C22) H(C11)	2.623	
C(C22) C(C31)	2.979(	22)
C(C22) C(C41)	3.095(	23)
C(C23) C(C24)	1.382(	62)
C(C23) H(C21)	2.693	
C(C24) H(C21)	2.581	
C(C31) C(C32)	1.450(	20)
C(C31) N(C01)	1.532(	14)
C(C31) C(C41)	2.488(	19)
C(C31) H(C11)	2.503	
C(C31) C(C43)	2.556(	26)
C(C31) H(C41)	2.611	
C(C31) H(C11)	2.700	
C(C31) C(C42)	3.003(	24)
C(C32) C(C33)	1.617(	24)
C(C32) H(C34)	2.157	
C(C32) C(C34)	2.397(	27)
C(C32) N(C01)	2.522(	18)
C(C32) H(C11)	2.671	
C(C32) H(C11)	3.048	
C(C33) C(C34)	1.123(	29)
C(C33) H(C34)	1.634	
C(C33) H(C34)	1.007	
C(C41) H(C41)	1.060	
C(C41) C(C42)	1.413(	16)
C(C41) N(C01)	1.524(	13)
C(C41) H(C42)	1.982	
C(C41) C(C43)	2.460(	20)
C(C41) H(C11)	2.609	
C(C41) H(C12)	2.621	
C(C41) H(C11)	2.777	
C(C42) H(C42)	0.975	
C(C42) C(C43)	1.566(	20)
C(C42) H(C41)	2.096	
[illegible]	2.[illegible]87(	[illegible])
[illegible]	2.[illegible](	[illegible])

C(C42)	H(C11)	2.722	
C(C42)	H(C12)	2.833	
C(C43)	C(C44)	1.389(	24)
C(C43)	H(C42)	1.970	
C(C43)	H(C41)	2.750	
C(C44)	H(C42)	2.456	
N(1)	H(N1B)	1.011	
N(1)	H(N1A)	1.012	
N(1)	RH(2')	2.221(	6)
N(1)	H(B 6')	2.666	
N(1)	H(B 5)	2.724	
N(1)	H(B 4)	2.736	
N(1)	H(BR)	2.763(	72)
N(1)	H(B 6)	2.951	
N(1)	RH(2)	3.002(	6)
N(2)	H(N2A)	0.955	
N(2)	H(N2B)	1.025	
N(2)	RH(2)	2.220(	6)
N(2)	H(B 6)	2.635	
N(2)	H(B 4')	2.864	
N(2)	H(B 3')	2.904	
N(2)	H(B 5')	2.980	
N(2)	RH(2')	3.013(	6)
N(2)	H(BR)	3.029(	72)
N(2)	H(B 6')	3.037	
N(C01)	H(C41)	2.025	
N(C01)	H(C31)	2.090	
N(C01)	H(C11)	2.096	
N(C01)	H(C21)	2.124	
N(C01)	H(C12)	2.799	
N(C01)	H(C42)	2.800	
N(C01)	H(C12)	2.811	
P(1)	RH(2)	2.367(	3)
P(1)	H(B 7)	2.710	
P(1)	H(BR)	2.854(	72)
P(2)	RH(2')	2.356(	2)
P(2)	H(B 7')	2.767	
P(2)	H(N1B)	2.791	
P(2)	H(BR)	2.870(	72)
RH(2')	H(BR)	1.923(	71)
RH(2')	H(N1B)	2.672	
RH(2')	H(B 6')	2.722	
RH(2')	H(N1A)	2.741	
RH(2')	H(B 3')	2.781	
RH(2')	H(B11')	2.866	
RH(2')	H(B 7')	2.934	
RH(2')	RH(2)	2.998(	1)
RH(2)	H(BR)	1.905(	71)

BOND ANGLES

FROM	THRU	TO	ANGLE	
H(B 3)	B(3)	C(1)	115.76	
H(B 3)	B(3)	B(2)	122.74	
H(B 3)	B(3)	B(4)	10[illegible]	
H(B 3)	B(3)	B(7)	13[illegible].97	
H(B 3)	B(3)	RH(2)	11[illegible]	
C(1)	B(3)	B([illegible])	104.4[illegible]	[illegible]
C(1)	B(3)	B([illegible])	[illegible]	[illegible]
C(1)	B(3)	B(7)	10[illegible]	[illegible]
C(1)	B(3)	RH([illegible])	[illegible]	[illegible]
B(2)	B(3)	B(4)	5[illegible]	[illegible]
B(2)	B(3)	B(7)	[illegible]	[illegible]
B(9)	B(3)	RH(2)	12[illegible]	
B(4)	B(3)	B(7)	10[illegible]	[illegible]
B(4)	B(3)	RH(2)	11[illegible]	[illegible]
B(7)	B(3)	RH(2)	[illegible]	[illegible]
H(B 3)	B(3)	C(1)	11[illegible]	
H(B 3)	B(3)	B(2)	1[illegible]	
H(B 3)	B(3)	B(4)	10[illegible]	
H(B 3)	B(3)	B(7)	13[illegible]	
H(B 3)	B(3)	RH(2)	[illegible]	
C(1)	B(3)	B(8)	102.9[illegible]	[illegible]
C(1)	B(3)	B(4)	56.3[illegible]	[illegible]
C(1)	B(3)	B(7)	104.7[illegible]	[illegible]
C(1)	B(3)	RH(2)	68.00[illegible]	[illegible]
B(8)	B(3)	B(4)	5[illegible]	[illegible]
B(8)	B(3)	B(7)	5[illegible]	[illegible]
B(8)	B(3)	RH(2)	11[illegible]	[illegible]
B(4)	B(3)	B(7)	106.[illegible]	[illegible]
B(4)	B(3)	RH(2)	1[illegible]	[illegible]
B(7)	B(3)	RH(2)	[illegible]	[illegible]
H(B 4)	B(4)	C(1)	1[illegible]	
H(B 4)	B(4)	B(9)	124.[illegible]	
H(B 4)	B(4)	B(5)	11[illegible]	
H(B 4)	B(4)	B(8)	124.50	
H(B 4)	B(4)	B(3)	119.[illegible]	
C(1)	B(4)	B(9)	107.07[illegible]	[illegible]
C(1)	B(4)	B(5)	59.48[illegible]	[illegible]
C(1)	B(4)	B(8)	106.69[illegible]	[illegible]
C(1)	B(4)	B(3)	60.07[illegible]	[illegible]
B(9)	B(4)	B(5)	60.45[illegible]	[illegible]
B(9)	B(4)	B(8)	60.7[illegible]	[illegible]
B(9)	B(4)	B(3)	109.1[illegible]	[illegible]
B(5)	B(4)	B(8)	108.9[illegible]	[illegible]
B(5)	B(4)	B(3)	109.1[illegible]	[illegible]
B(5)	B(4)	H(B 4)	127.7[illegible]	
B(8)	B(4)	B(3)	59.[illegible]	[illegible]
H(B 4)	B(4)	C(1)	110.[illegible]	
H(B 4)	B(4)	B(8)	134.76	
H(B 4)	B(4)	B(9)	132.3[illegible]	
H(B 4)	B(4)	B(5)	114.2[illegible]	
H(B 4)	B(4)	B(3)	118.[illegible]	
C(1)	B(4)	B(7)	105.[illegible]	6[illegible]
C(1)	B(4)	B(9)	104.[illegible]	[illegible]
[illegible]	B(4)	B(5)	59.20[illegible]	5[illegible]
[illegible]	B(4)	B(3)	[illegible]9.[illegible]	[illegible]
[illegible]	B(4)	B([illegible])	[illegible]	[illegible]
[illegible]	[illegible]	B([illegible])	[illegible]	[illegible]
[illegible]	[illegible]	B([illegible])	[illegible]	[illegible]
[illegible]	[illegible]	B([illegible])	[illegible]	[illegible]

B(9)	B(4)	B(3)	107.8[illegible]	[illegible]
B(5)	B(4)	B(3)	108.7[illegible]	75)
H(B 5	B(5)	C(1)	120.70	
H(B 5)	B(5)	B(10)	120.8[illegible]	
H(B 5	B(5)	B(4	127.4[illegible]	
H(B 5)	B(5)	B([illegible]	[illegible]	
H(B 5	B(5)	B([illegible]	114.[illegible]	
C(1)	B(5)	B(10)	105.[illegible]	41
C(1)	B(5)	B([illegible]	59.20(	[illegible]
C(1)	B(5)	B([illegible]	104.22(	[illegible]
C(1)	B(5)	B(6)	58.97(	[illegible]
B(10)	B(5)	B(4)	107.6[illegible]	[illegible]
B(10)	B(5)	B(9	[illegible]8.52(	[illegible]
B(10)	B(5)	B(6	55.72(	[illegible]
B(4)	B(5)	B([illegible]	55.42(	[illegible]
B(4)	B(5)	B([illegible]	107.69(	[illegible]
B(9)	B(5)	B([illegible]	108.[illegible]	[illegible]
H(B [illegible]	B(5	C(1	109.[illegible]	
H(B [illegible]	B(5)	B(10)	[illegible]4[illegible]	
H(B [illegible]	B(5	B(6)	122.[illegible]	
H(B [illegible]	B([illegible]	B([illegible]	130.40	
H(B [illegible]	B([illegible]	B([illegible]	[illegible]	
C(1)	B([illegible]	B(10)	100.[illegible]	[illegible]
C(1)	B([illegible]	B([illegible]	[illegible]	[illegible]
C(1)	B(3)	B([illegible]	104.[illegible]	[illegible]
C(1)	B([illegible]	B(4	60.49(	[illegible]
B(10)	B([illegible]	B(6)	5[illegible].65(	[illegible]
B(10)	B([illegible]	B(9)	[illegible]	[illegible]
B(10)	B(5)	B(4)	107.[illegible]	[illegible]
B(6)	B(5)	B(9)	108.7[illegible]	[illegible]
H(B 6	B(6)	C(1)	117.2[illegible]	
H(B 6)	B(6)	B(10)	125.[illegible]	
H(B 6	B(6)	B(4)	117.[illegible]	
H(B 6)	B(6)	B([illegible]	127.[illegible]	
H(B 6	B(6)	RH([illegible]	100.00	
C(1	B(6)	B(10)	102.0[illegible]	[illegible]
C(1)	B(6)	B([illegible]	56.[illegible]	[illegible]
C(1)	B(6)	B([illegible]	103.[illegible]	[illegible]
C(1)	[illegible]	B([illegible]	[illegible]	[illegible]
B(10)	[illegible]	B([illegible]	[illegible]	[illegible]
B(10)	[illegible]	B(4)	5[illegible].9[illegible]	[illegible]
B(10)	B(6)	RH(2)	120.1[illegible]	[illegible]
B(5)	B(6)	B(1[illegible]	105.2[illegible]	[illegible]
B(5)	B(6)	RH(2)	119.7[illegible]	[illegible]
B(1[illegible]	B(6)	RH([illegible]	67.57(	40
H(B 6	B(6)	C(1)	117.08	
H(B 6	B(6)	B(1[illegible]	124.7[illegible]	
H(B 6)	B(6)	B(5)	117.[illegible]	
H(B 6	B(6)	B(11)	126.7[illegible]	
H(B 6	B(6)	RH(2)	106.9[illegible]	
C(1)	B(6)	B(10)	105.11(	7[illegible]
C(1)	B(6)	B(5)	58.94(	5[illegible]
C(1)	B(6)	B(11)	108.20(	7[illegible]
C(1)	B(6)	RH(2)	66.58(	4[illegible]
B(10)	B(6)	B(5)	59.[illegible]	[illegible]
B(10)	B(6)	B(11)	60.47(	[illegible]
B(10)	B(6)	RH(2)	117.[illegible]	[illegible]
B(5)	B(6)	B(11)	109.04(	7[illegible]
B(5)	B(6)	RH(2)	1[illegible]9.[illegible]	[illegible]
B(11)	B(6)	RH([illegible]	[illegible].9[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	114[illegible]	
[illegible]	[illegible]	[illegible]	[illegible]	
[illegible]	[illegible]	[illegible]	[illegible]	

H(B 7)	B(7)	B(11)	128.19	
H(B 7)	B(7)	RH(2)	119.72	
H(B 7)	B(7)	B(8)	62.22	
B(8)	B(7)	B(12)	57.23	[illegible]
[illegible]	B(7)	B(3)	57.[illegible]	[illegible]
[illegible]	B(7)	B(11)	106.[illegible]	[illegible]
B(8)	B([illegible])	RH(2)	[illegible]	[illegible]
B(12)	B(7)	B([illegible])	[illegible]	[illegible]
[illegible]	B(7)	B(11)	[illegible]	[illegible]
[illegible]	B(7)	RH(2)	[illegible]	[illegible]
[illegible]	B(7)	B(11)	[illegible]	[illegible]
[illegible]	B(7)	RH(1)	[illegible]	[illegible]
B(11)	B([illegible])	RH(1)	[illegible]	[illegible]
H(B 7)	B(7)	B(3)	117.[illegible]	
H(B 7)	B(7)	B(12)	120.[illegible]	
H(B 7)	B(7)	B([illegible])	120.[illegible]	
H(B 7)	B(7)	B(11)	120.[illegible]	
H(B 7)	B(7)	RH(	112.[illegible]	
B(8)	B(7)	B(12)	6[illegible]	[illegible]
B(8)	B(7)	B(3)	60.0[illegible]	[illegible]
B(8)	B(7)	B(11)	107.[illegible]	[illegible]
B(8)	B(7)	RH(2)	11[illegible]	[illegible]
B(12)	B(7)	B(3)	107.[illegible]	[illegible]
B(12)	B(7)	B(11)	58.79	[illegible]
B(12)	B(7)	RH(2)	118.6[illegible]	[illegible]
B(3)	B(7)	B(11)	107.7[illegible]	[illegible]
B(3)	B(7)	RH(2)	67.89	[illegible]
B(11)	B(7)	RH(2)	67.78	[illegible]
H(B 8)	B(8)	B(4)	119.[illegible]	
H(B 8)	B(8)	B(12)	121.[illegible]	
H(B 8)	B(8)	B(3)	124.1[illegible]	
H(B 8)	B(8)	B(9)	116.[illegible]	
H(B 8)	B(8)	B(7)	125.0[illegible]	
B(4)	B(8)	B(12)	10[illegible]	[illegible]
B(4)	B(8)	B(3)	61.1[illegible]	[illegible]
B(4)	B(8)	B(9)	59.[illegible]	[illegible]
B(4)	B(8)	B(7)	104.80	[illegible]
B(12)	B(8)	B(3)	108.4[illegible]	[illegible]
B(12)	B(8)	B(9)	59.[illegible]	[illegible]
B(12)	B(8)	B(7)	60.55	5[illegible]
B(3)	B(8)	B(9)	109.16	[illegible]
B(3)	B(8)	B(7)	61.1[illegible]	4[illegible]
B(9)	B(8)	B(7)	109.14	6[illegible]
H(B 9)	B(9)	B(7)	119.3[illegible]	
H(B 9)	B(9)	B(12)	121.7[illegible]	
H(B 9)	B(9)	B([illegible])	122.1[illegible]	
H(B 9)	B(9)	B(4)	121.[illegible]	
H(B 9)	B(9)	B([illegible])	120.[illegible]	
B(7)	B(9)	B(12)	60.6[illegible]	7[illegible]
B(7)	B(9)	B([illegible])	108.[illegible]	[illegible]
B(7)	B(9)	B(4)	110.[illegible]	[illegible]
B(7)	B(9)	B([illegible])	61.67	[illegible]
B(12)	B(9)	B([illegible])	58.[illegible]	[illegible]
B(12)	B(9)	B(4)	108.[illegible]	[illegible]
[illegible]	B(9)	B([illegible])	109.[illegible]	[illegible]
[illegible]	B(9)	B(4)	60.6[illegible]	[illegible]
[illegible]	B(9)	B([illegible])	108.[illegible]	[illegible]
[illegible]	B(9)	B([illegible])	60.77	6[illegible]
[illegible]	[illegible]	B([illegible])	123.60	
[illegible]	[illegible]	B([illegible])	124.[illegible]	
[illegible]	[illegible]	B([illegible])	11[illegible]	
[illegible]	[illegible]	B([illegible])	[illegible]	
[illegible]	[illegible]	B([illegible])	[illegible]	

B(12)	B(9)	B(4)	107.42(	[illegible]
B(12)	B(9)	B(10)	60.[illegible]	[illegible]
B(12)	B(9)	B(5)	107.[illegible]	[illegible]
B(12)	B(9)	B(8)	[illegible]	[illegible]
B(1)	B(9)	B(10)	107.[illegible]	[illegible]
B(4)	B(9)	B(5)	[illegible].24(	[illegible]
B(4)	B(9)	B(8)	59.7[illegible]	[illegible]
B(10)	B(9)	B(5)	60.3[illegible]	[illegible]
B(10)	B(9)	B(8)	107.2[illegible]	66
B(5)	B(9)	B(8)	107.[illegible]	[illegible]
H(B 9)	B(9)	B(10)	124.[illegible]	
H(B 9)	B(9)	B(12)	124.[illegible]	
H(B 9)	B(9)	B(5)	[illegible]	
H(B 9)	B(9)	B(8)	[illegible]	
H(B 9)	B(9)	B(4)	10[illegible]	
B(10)	B(9)	B(12)	[illegible]	[illegible]
B(10)	B(9)	B(4)	[illegible]	[illegible]
B(10)	B(9)	B(8)	10[illegible]	[illegible]
B(10)	B(9)	B(4)	10[illegible]	[illegible]
B(12)	B(9)	B(5)	110.[illegible]	[illegible]
B(12)	B(9)	B(9)	60.[illegible]	[illegible]
B(12)	B(9)	B(4)	10[illegible]	[illegible]
B(8)	B(9)	B(8)	109.[illegible]	7[illegible]
B(8)	B(9)	B(4)	[illegible]	[illegible]
B(8)	B(9)	B(4)	60.[illegible]	[illegible]
H(B10)	B(10)	B(5)	125.[illegible]	
H(B10)	B(10)	B(5)	[illegible]	
H(B10)	B(10)	B(9)	[illegible]	
H(B10)	B(10)	B(12)	[illegible]	
H(B10)	B(10)	B(11)	[illegible]	
B(9)	B(10)	B(6)	[illegible]	[illegible]
B(9)	B(10)	B(9)	[illegible]	
B(9)	B(10)	B(12)	106.[illegible]	
B(6)	B(10)	B(11)	[illegible]	[illegible]
B(5)	B(10)	B(9)	110.[illegible]	[illegible]
B(5)	B(10)	B(12)	108.[illegible]	[illegible]
B(5)	B(10)	B(11)	61.[illegible]	[illegible]
B(9)	B(10)	B(12)	59.[illegible]	[illegible]
B(9)	B(10)	B(11)	110.10(	[illegible]
B(12)	B(10)	B(11)	60.[illegible]	[illegible]
H(B10)	B(10)	B(9)	1[illegible]	
H(B10)	B(10)	B(6)	1[illegible]	
H(B10)	B(10)	B(5)	120.[illegible]	
H(B10)	B(10)	B(12)	117.[illegible]	
H(B10)	B(10)	B(11)	10[illegible]	
B(9)	B(10)	B(6)	109.7[illegible](	[illegible]
B(9)	B(10)	B(5)	6[illegible].[illegible](	7[illegible]
B(9)	B(10)	B(12)	59.05(	7[illegible]
B(9)	B(10)	B(11)	109.[illegible](	[illegible]
B(6)	B(10)	B(5)	60.4[illegible]	6[illegible]
B(6)	B(10)	B(12)	108.79(	76
B(4)	B(10)	B(11)	6[illegible].[illegible]	6[illegible]
B(5)	B(10)	B(12)	109.64(	[illegible]
B(5)	B(10)	B(11)	112.05(	7[illegible]
B(12)	B(10)	B(11)	60.04(	7[illegible]
H(B11)	B(11)	B(10)	119.35	
H(B11)	B(11)	B(12)	117.13	
H(B11)	B(11)	B(6)	126.35	
H(B11)	B(11)	B(7)	121.50	
H(B11)	B(11)	BH(2)	1[illegible]	
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H(B11)	B(11)	B(6)	121.84	
H(B11)	B(11)	B(7)	12[illegible]	
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B(12)	B(11)	B(7)	[illegible]	[illegible]
B(12)	B(11)	RH(2)	[illegible]	
B(10)	B(11)	B(6)	[illegible]	[illegible]
B(10)	B(11)	B(7)	105.70	[illegible]
B(10)	B(11)	RH(2)	11[illegible].70	[illegible]
B(6)	B(11)	B(7)	10[illegible]	
B(6)	B(11)	RH(2)	[illegible]	[illegible]
B(7)	B(11)	RH(2)	64.[illegible]	
H(B12)	B(12)	B(9)	12[illegible]	
H(B12)	B(12)	B(10)	127.00	
H(B12)	B(12)	B(8)	120.6[illegible]	
H(B12)	B(12)	B(11)	116.94	
H(B12)	B(12)	B(7)	11[illegible]	
B(9)	B(12)	B(10)	60.1[illegible]	[illegible]
B(9)	B(12)	B(8)	60.7[illegible]	[illegible]
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B(9)	B(12)	B(7)	110.3[illegible]	[illegible]
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B(9)	B(12)	B(11)	109.[illegible]	[illegible]
B(9)	B(12)	B(7)	10[illegible]	[illegible]
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B(11)	B(12)	B(7)	62.40	[illegible]
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B(6)	C(1)	RH(2)	67.54(	[illegible]
B(5)	C(1)	B(3)	112.44(	[illegible]
B(5)	C(1)	RH(2)	124.0[illegible](	[illegible]
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B(4)	C(1)	B(5)	6[illegible].71(	[illegible]
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H(C12)	C(C12)	C(C13)	104.[illegible]	
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H(C21)	C(C21)	C(C22)	106.62	
H(C21)	C(C21)	N(C01)	10[illegible].97	
C(C22)	C(C21)	N(C01)	116.64(	[illegible]
C(C21)	C(C22)	C(C23)	111.30(	[illegible]
C(C24)	C(C23)	C(C22)	94.5[illegible](	[illegible]
C(C32)	C(C31)	N(C01)	115.40(	[illegible]
C(C31)	C(C32)	C(C33)	111.48(	[illegible]
C(C34)	C(C33)	C(C32)	120.29(	[illegible]
H(C34)	C(C34)	C(C33)	99.42	
H(C41)	C(C41)	C(C42)	11[illegible]	
H(C41)	C(C41)	N(C01)	10[illegible]	
C(C42)	C(C41)	N(C01)	116.5[illegible](	[illegible]
H(C42)	C(C42)	C(C41)	110.[illegible]1	
H(C42)	C(C42)	C(C43)	[illegible]	
C(C41)	C(C42)	C(C43)	111.2[illegible](	[illegible]
C(C44)	C(C43)	C(C42)	114.4[illegible](	[illegible]
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H(N2B)	N(2)	RH(2)	114.6[illegible]	
C(12)	N(2)	RH(3)	110.5[illegible]	4[illegible]
C(C11)	N(C01)	C(C41)	1[illegible]	[illegible]
C(C11)	N(C01)	C(C[illegible])	110.[illegible]	[illegible]
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C(C41)	N(C01)	C([illegible])	10[illegible]	[illegible]
C(C71)	N(C01)	C(C[illegible])	[illegible]	
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H(BR)	RH(2)	[illegible]	[illegible]	[illegible]
H(BR)	RH(2)	[illegible]	[illegible]	[illegible]
H(BR)	RH(2)	N(1)	[illegible]	
H(BR)	RH(2)	B(11)	[illegible]	[illegible]
H(BR)	RH(2)	[illegible]	[illegible]	
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		[illegible]	[illegible]	
		[illegible]		

B(7)	RH(2)	N(2)	144.23(35)
B(7)	RH(2)	B(5)	82.30(40)
B(7)	RH(2)	B(11)	48.61(40)
B(7)	RH(2)	P(1)	83.26(38)
B(7)	RH(2)	RH(2')	144.72(32)
N(2)	RH(2)	B(6)	83.99(31)
N(2)	RH(2)	B(11)	98.96(34)
N(2)	RH(2)	P(1)	93.70(17)
N(2)	RH(2)	RH(2')	68.70(16)
B(6)	RH(2)	B(11)	48.02(40)
B(6)	RH(2)	P(1)	151.61(28)
B(6)	RH(2)	RH(2')	92.81(26)
B(11)	RH(2)	P(1)	104.97(38)
B(11)	RH(2)	RH(2')	140.66(30)
P(1)	RH(2)	RH(2')	112.80(6)

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The reaction of $RhCl(PPh_3)_3$ with nido-$B_{10}H_{12}CNH_3$ in the presence of $[(n\text{-}C_4H_9)_4N]OH$ produced $[(n\text{-}C_4H_9)_4N]$[closo-2,2-$(Ph_3P)_2$-2-H-1-(NH_2)-2,1-$RhCB_{10}H_{10}$], which upon heating in methanol produced a new orange compound confirmed by an X-ray diffraction study to be the $[(n\text{-}C_4H_9)_4N]^+$ salt or an-NH_2-bridged Rh-H-Rh dimer anion.

APPENDIX

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